1-Pentanol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.36

Global applicability domain: Inside

Local applicability domain index: 7.96e-01

Confidence level: 8.47e-01

Nearest Neighbors from the Training Set

Image not found
1-Pentanol
Measured: 1.51
Predicted: 1.36

Image not found
2-Methyl-1-butanol
Measured: 1.29
Predicted: 1.26

Image not found
Isopentyl alcohol
Measured: 1.16
Predicted: 1.24

Image not found
3-Pentanol
Measured: 1.21
Predicted: 1.21

Image not found
Pentan-2-ol
Measured: 1.19
Predicted: 1.21